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BATPAC MODEL DEVELOPMENT



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Project Title: Core BatPaC Development and Implementation, Project ID: ES228

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OVERVIEW

Timeline

- Start: 2012
- End: 2017

Budget

- FY14: 575K
- FY15: 575K
- FY16: 575K

Barriers

To the development of PHEV and EV batteries that meet or exceed DOE/USABC goals

- Cost
- Performance

Collaborations / Interactions

- U.S. Environmental Protection Agency, Volpe-USDOT
- B&W MEGTEC, GM, LGChem, PPG, PEC-NA, Maccor, Paraclete, Miltec, Lambda Technologies, Navitas, Cummins, Ricardo, Rio Tinto, ORNL, NREL

RELEVANCE

- This modeling effort supports projects through the development and utilization of efficient simulation, analysis, and design tools for advanced lithium ion battery technologies
 - Enables assessment of technology developments at the pack level
- The EPA uses BatPaC to predict the cost of battery technologies for their 2017-2025 rule making
 - Argonne updates BatPaC with cost inputs, modification of constraints, studies* of variable factory utilization, etc.
- BatPaC is the only peer-reviewed LIB design and cost model available in the public domain

*Nelson, P.A., et al., “Cost savings for manufacturing lithium batteries in a flexible plant,” Journal of Power Sources, Volume 283, 1 June 2015, Pages 506–516

OBJECTIVES AND IMPACT

- Objective: Develop and utilize efficient simulation and design tools for Li-ion batteries to predict
 - Battery pack metrics (size, weight, etc.) from laboratory data
 - Cost of battery packs when manufactured in large volume
- Benefit to DOE
 - Support assessments of ongoing and proposed technologies through projections of cost and performance at the pack level
 - Project material and energy demands
 - Identify opportunities for cost reduction in manufacturing process

APPROACH

- Design a battery based on the power and energy specifications for a given cell chemistry
 - Sizes the battery components to meet the specifications
 - Tracks all the materials used in the pack
 - Cost based on a described manufacturing process
- Reduce uncertainty in model predictions
 - Update the default chemistries, their properties, and material and processing costs
 - Develop higher fidelity models of the physical and electrochemical phenomenon, and manufacturing flow path (quantify energy needs)
 - Validate results with OEMS, manufacturers, component developers

PROGRESS

Milestones / Status

- ✓ Release new version of BatPaC
 - due December 2015
 - Status: Complete
 - Revised manual in preparation

- Initiate study on volume expansion
 - due March 2016
 - Status: In progress

- ✓ Update energy/utility demands in battery manufacture
 - due June 2016
 - Status: Models set up for dry room, cathode drying, NMP recovery, cathode material production

- ✓ Develop improved cost model for production of cathode material
 - due September 2016
 - Status: Met

OUTLINE OF TECHNICAL ACCOMPLISHMENTS

Higher fidelity spreadsheet models have been set up to review and update input data in BatPaC

1. Optimum electrode loading – calculated from an analytical expression derived from experimental data and transport modeling
2. NMC cathode production – Energy & cost estimates with process model
3. Cathode drying, NMP recovery – Energy & cost estimates with process model
4. Dry Room – Energy & cost estimates with process model
5. Formation cycling – Energy & cost estimates using process model
6. Included table reporting the inventory of materials in the battery pack
7. BatPaC Version 3.0 Released
 - 1) Calculates time required for fast charging of EV batteries
 - 2) Material costs updated
 - 3) Revised electrode thickness calculations
 - 4) Added option to use a blend of LMO-NMC cathode
 - 5) Material and processing costs updated with calculations from 1, 2, 3

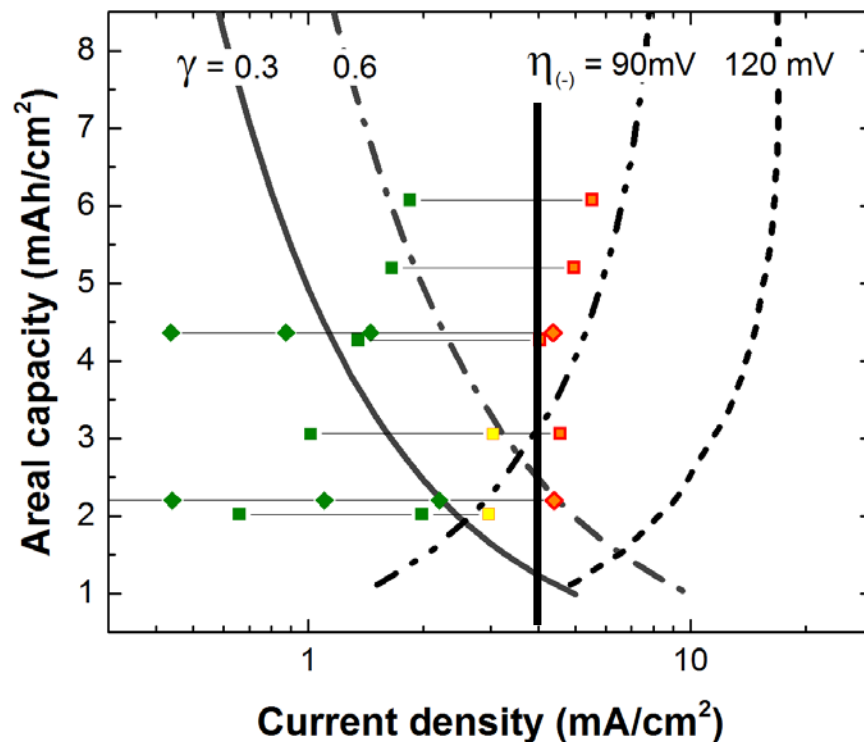
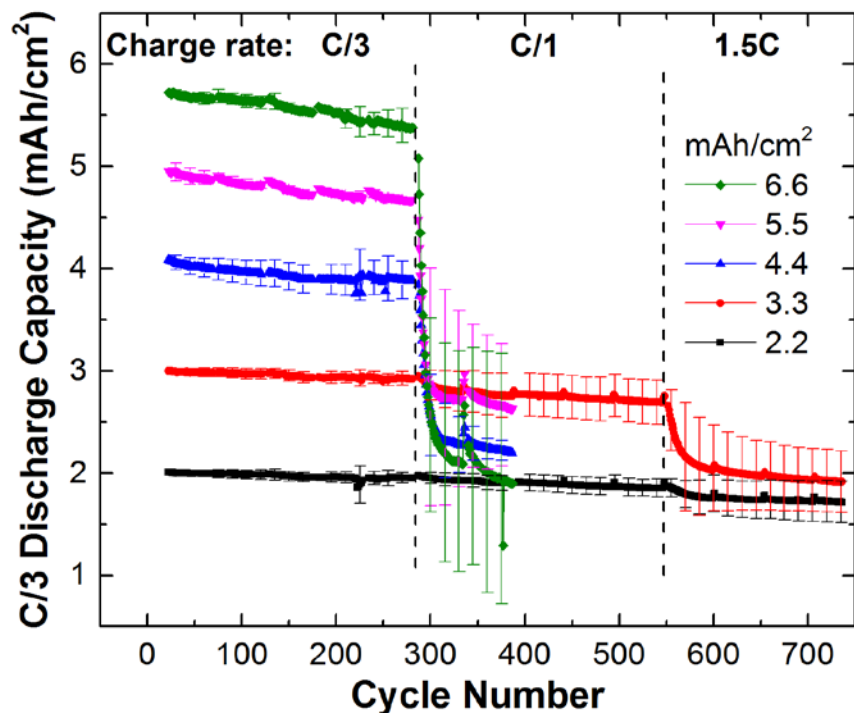
TECHNICAL ACCOMPLISHMENT

OPTIMUM ELECTRODE THICKNESS

Analytical expression for limitations on both discharge & charge

NMC622/Gr 14 cm² pouch cells
C/3 discharge rate; charge varied

$$Q_A = \sqrt{\frac{\gamma Q_v \left(\frac{\varepsilon}{\tau} \right) D c F t_d}{(1 - t_+^o)}}$$



4 mA/cm² is a critical current density to be avoided during charge

TECHNICAL ACCOMPLISHMENT INCLUDED CALCULATIONS FOR FAST CHARGING EV BATTERY

Calculates time required to add 60-80% to SOC

- Identifies limiting charging restriction
 - Li deposition
 - Power of charger
 - Insufficient cooling
- Batt-1 positive electrode thickness limited by sustained discharge
- Batt-2 positive electrode thickness reduced to 70 μm to improve charging time
- Batt-3 positive electrode thickness further reduced but at higher cost

	<i>Batt-1</i>	<i>Batt-2</i>	<i>Batt-3</i>
Energy storage, kWh	79.4	79.4	79.4
Capacity at C/3, Ah	301	299	300
Battery Power at 80% OCV, kW	302	393	419
Positive Electrode thickness, μm	94	70	65
Max. current density to avoid lithium deposition, mA/cm^2	4	4	4
Initial battery temperature, $^{\circ}\text{C}$	15	15	15
Max. allowed battery temperature, $^{\circ}\text{C}$	40	40	40
Fast charge limiting condition	Li dep.	Li dep.	Temp.
Time to add 60% of SOC (15-75%)	37	27	25
Time to add 80% of SOC (15-95%)	45	33	31
Battery cost to OEM, \$	10,090	10,660	10,840

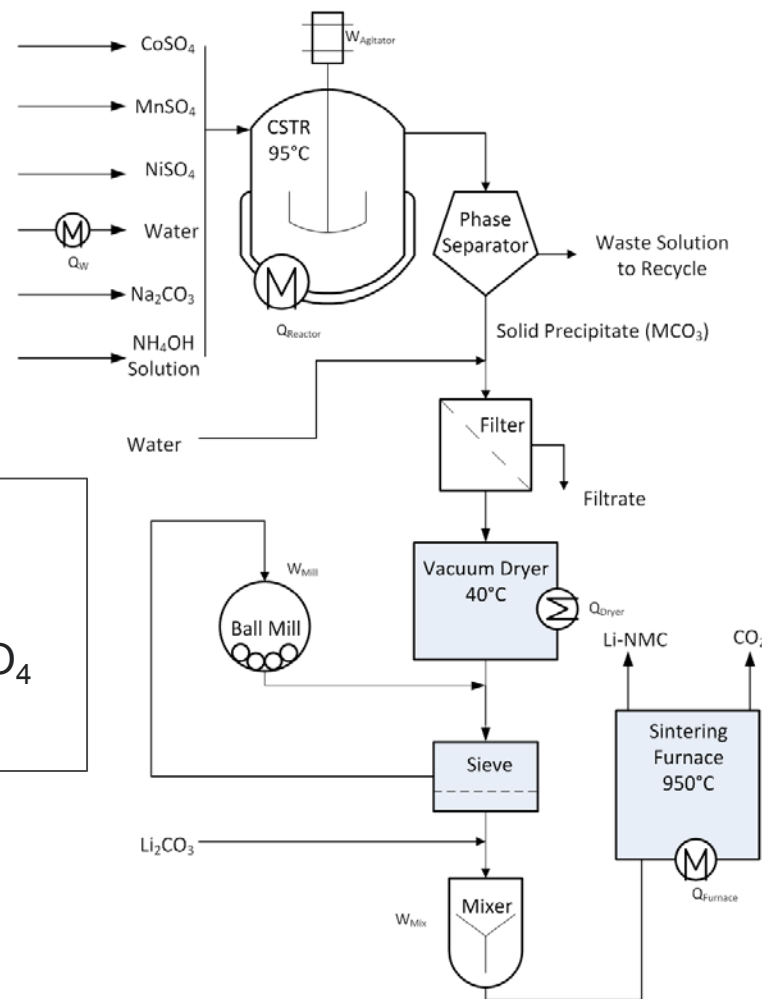
TECHNICAL ACCOMPLISHMENT MODELED NMC PRODUCTION PROCESS

Estimated production cost of NMC333 is ~\$20 per kg

- $\text{MSO}_4 + \text{Na}_2\text{CO}_3 = \text{MCO}_3\downarrow + \text{Na}_2\text{SO}_4$
 - The energy demand is ~ 2 kWh/kg
 - Thermal/Electrical = 3
 - Raw materials contribute 50+% to cost of final product
 - NMC622 cost estimated at \$18/kg
- $\text{MSO}_4 + 2\text{NaOH} = \text{M}(\text{OH})_2\downarrow + \text{Na}_2\text{SO}_4$
 - Requires more water, costs 40 ¢/kg more

Assumptions

- 4000 kg/day plant capacity
- Assumed prices, \$/kg of M (commodity price)
 - Cost of 58.7 kg of Ni = Cost of 139 kg of NiSO_4
 - Ni=\$9.9, Mn=\$1.8, Co=\$27.8 (Oct.2015)

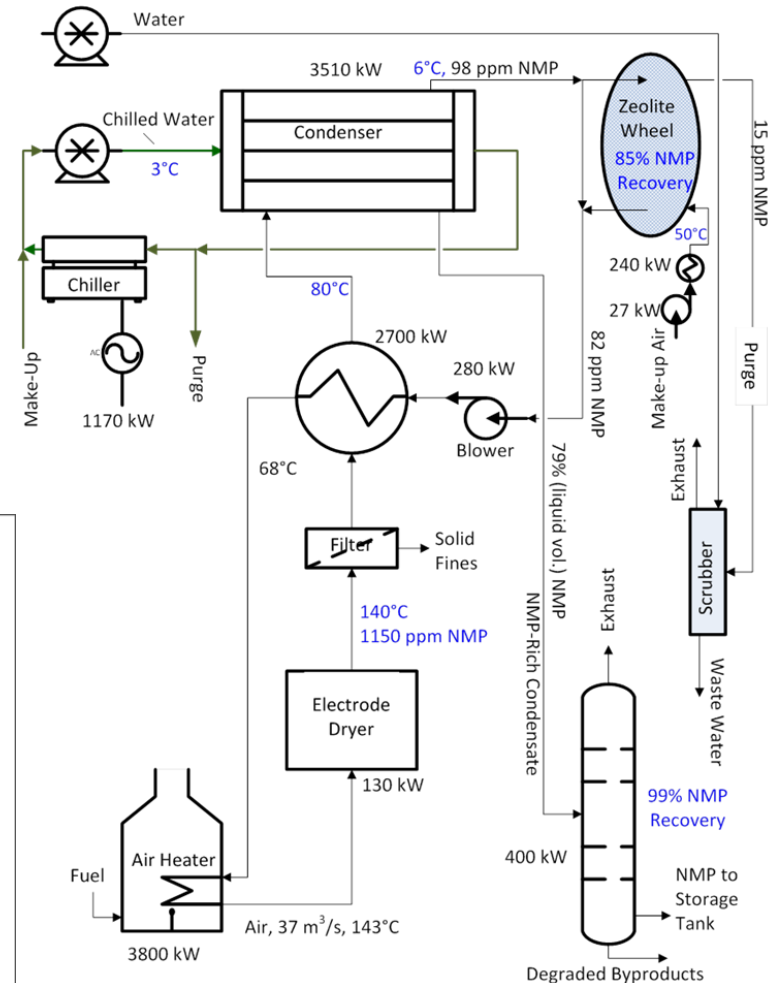
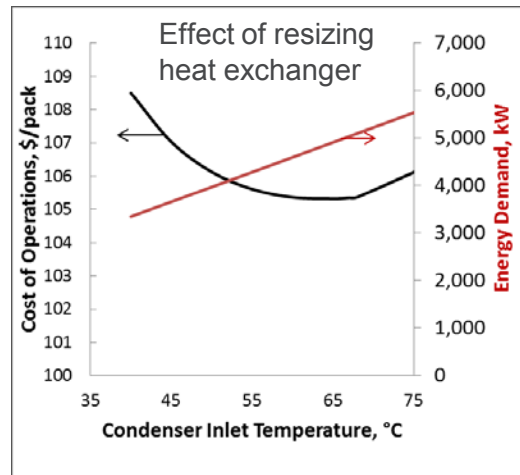


- Feb.2016 prices: Ni=\$8.7, Mn=\$1.5, Co=\$22.5, cost of NMC333=\$18 per kg

TECHNICAL ACCOMPLISHMENT MODELED CATHODE DRYING AND NMP RECOVERY

Cathode drying and recovery contributes ~\$10 / kWh (3%) to the cost of a PHEV battery pack

- The process requires ~420 kWh per kWh battery pack*
– 5800 kW, 580 kW/kWh
- Energy demand is 45 times the energy needed for NMP vaporization
- Large energy demand is constrained by safety
– Large excess air is needed to limit NMP concentration in hot air
- The air heater for the coating line ovens (dryer) is the largest contributor with 60+% of total demand
- Cost of energy is ~10% of process, with opportunities to reduce energy demand (CO₂-equivalent emissions)

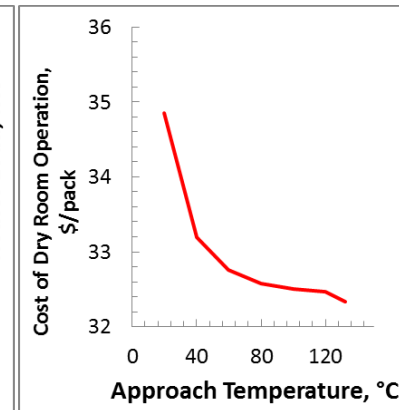
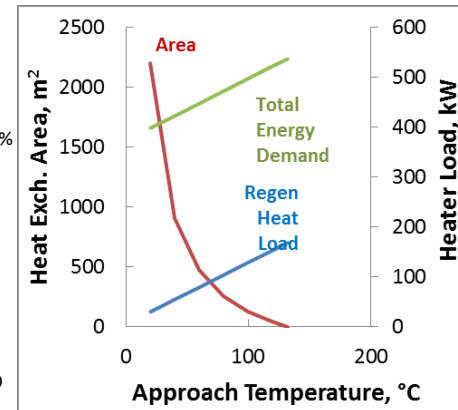
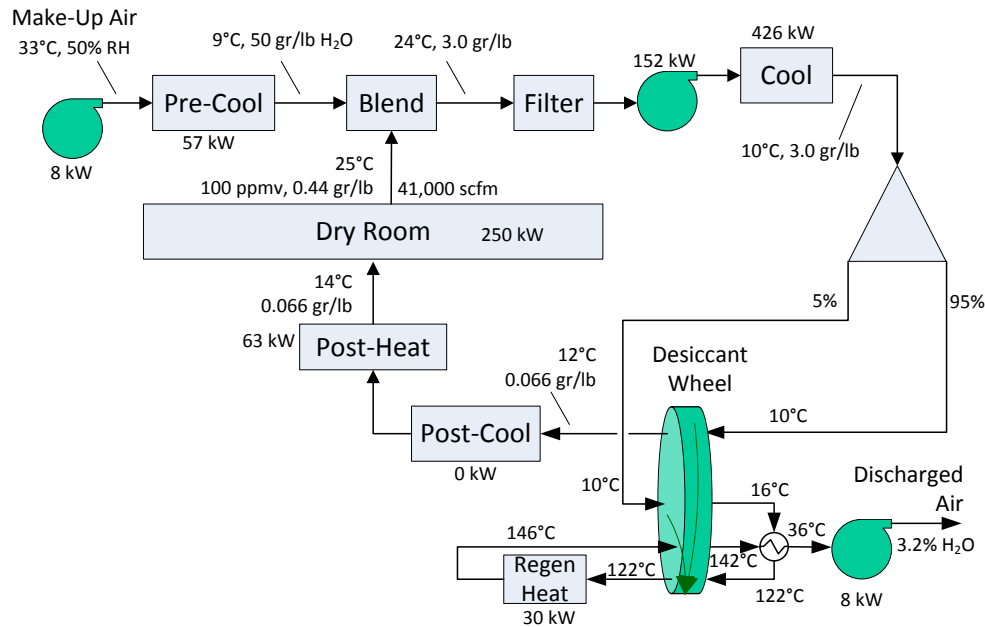


*Plant producing 100K packs/yr of 60 kWh, 10 kWh PHEV batteries

**Process for evaporation and recovery
of 4M kg/yr of NMP**

TECHNICAL ACCOMPLISHMENT MODELED THE AIR TREATMENT FOR THE DRY ROOM

Contributes \$35 (~1%) to the cost of each battery pack*



- The process consumes 400 kW for a 16,000 m³ dry room*
- Cost of energy (electric + natural gas) represents 5% of the cost of operations
- Eliminating the heat exchanger reduces capital cost but increases energy demand
- Sensor controlled air rates will lower air flow rates and reduce energy and cost

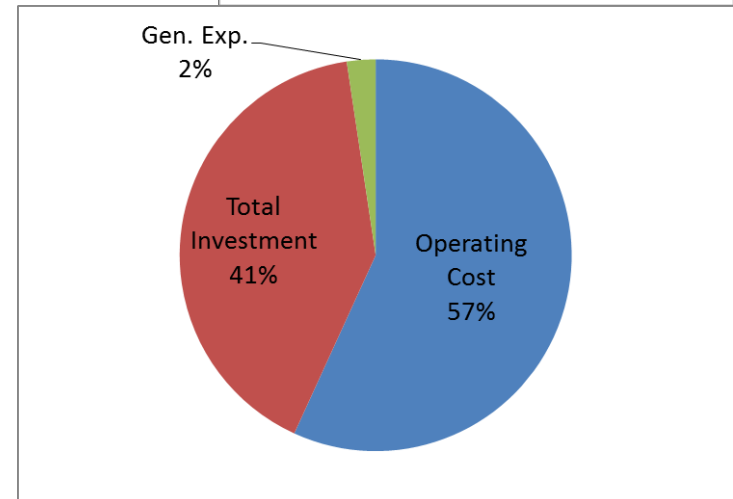
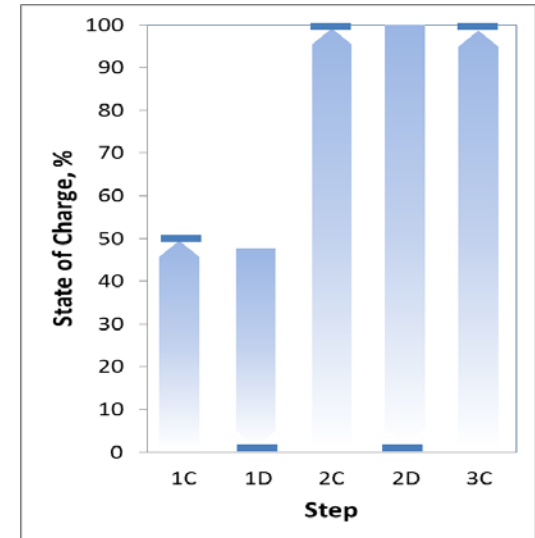
TECHNICAL ACCOMPLISHMENT MODELED THE FORMATION CYCLING PROCESS

Contributes \$90 (3%) to the cost of the battery pack

- Basis: 100K pks/year, 10.1 M cell/yr
 - 10 kWh PHEV, 29 Ah
- Energy demand
 - Electrical energy (charging)
 - 3600 MWh/year, 500 kW, 50 kW/kWh
- Heat generated during charge/discharge
 - 240 MWh/year, 33 kW
- Heat generated if discharged energy dumped to load
 - 1900 MWh/year, 265 kW

Preliminary Estimates

- Floor Space: 900 m²
- Cost Contribution: \$9 per kWh
 - Cost of electricity ~ 1% of annual cost
 - Large number of cyclers and racks represent a large fraction of the capital equipment cost
 - Eliminating one full charge/discharge step can reduce cost by 35%



TECHNICAL ACCOMPLISHMENT MATERIAL INVENTORY REPORT

- Variation in material content is small on a per kWh basis
- The fraction of active material content is higher in larger batteries
- Will be included in next BatPaC update

MATERIAL INVENTORY:

VARIATION IN MATERIALS CONTENT IS SMALL
WHEN NORMALIZED TO BATTERY CAPACITY

	<i>HEV</i>	<i>PHEV</i>	<i>EV</i>
Energy, kWh	4	12	62
Power, kW	120	60	180
Chemistry	LMO-G	LMO-G	NMC622-G
<i>Material</i>	<i>kg/kWh</i>		
Lithium	0.11	0.11	0.13
Nickel			0.61
Cobalt			0.19
Manganese	1.6	1.6	0.20
Aluminum	1.7	1.5	0.95
Copper	1.9	0.92	0.55
Graphite	1.0	1.0	1.1

COLLABORATION

Supported two agencies and several commercial organizations with BatPaC studies

- Incorporated suggestions from USEPA feedback to beta version
- Supported USDOT with cost projections
- Incorporated feedback from private companies
- Joint publication on drying with ORNL, B&W MEGTEC
- Provided calculations and support
 - PPG, Paraclete, Miltec, Ricardo, Rio Tinto, Northwestern U.
- Continuing discussions to extend and validate model
 - GM, LGChem, PEC-NA, Maccor, Lambda Technologies, Navitas, Cummins, Ricardo

PROPOSED FUTURE WORK

- Develop higher fidelity models of steps in the manufacturing and supply chain
 - Coaters, alternative drying, charge retention
 - Production of electrolytes (LiPF_6 , etc.), costly active materials
 - Validate results generated from BatPaC and supporting models
- Include volume expansion mitigation designs (foam or springs, etc.)
- Study impact of developing technologies
 - Coat electrodes without use of binder solvent
 - Plant automations for large plants (e.g., 500K EV per year)
- Support USEPA and USDOT

SUMMARY

The BatPaC spreadsheet tool is a resource for sponsors, technology assessors, and developers

- Projects impact of technology developments at component level to pack-level performance and cost
- BatPaC calculations and data reporting has been extended
 - Electrode thickness, materials inventory, etc.
- BatPaC input data is being refined with more detailed models and collaboration with experts
 - Supporting models calculate energy demands of the manufacturing process
 - The cathode drying and NMP recovery process is the most energy intensive
 - Identifies opportunities for cost reduction

Process (100K/year, 10 kWh PHEV)	Energy Demand
Drying and NMP Recovery	5800 kW
Production of NMC333	550 kW
Formation Cycling	500 kW
Dry Room Air Management	400 kW

<http://www.cse.anl.gov/batpac/>

RESPONSES TO PREVIOUS YEAR REVIEWERS' COMMENTS

- A reviewer asked for more details on how the fast charging work will be included in BatPaC.
 - *New worksheet added, which calculates the time needed to add to the SOC and identifies the constraint that limits faster charging.*
- A reviewer recommended looking more at sulfur
 - *Sulfur batteries will be included as the technology acceptance for automotive use. It is currently being reviewed^[1] and developed in other projects.*
- A reviewer noted that high-volume battery producers were conspicuously absent
 - *We are trying to reach more producers to review our methodology and calculations.*
- A reviewer commented that the cathode work is heavily weighted in this model and other components such as the anode and separator needs attention.
 - *The technologies being addressed are typically selected on the basis of performance or cost impact*

¹⁸
[1] Eroglu, D., et.al., Journal of the Electrochemical Society, 2015, 162 (6), A982-A990, doi: 10.1149/2.0611506jes

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TECHNICAL BACK-UP SLIDES

PUBLICATIONS

- Gallagher, K.G., et al, “Optimizing Areal Capacities Through Understanding The Limitations Of Lithium-ion Electrodes,” Journal of the Electrochem. Soc. 163(2) A138 (2016)
- Ahmed, S., Nelson, P.A., Dees, D.W., “Study of a Dry Room in a Battery Manufacturing Plant using a Process Model,” submitted to the Journal of Power Sources, Nov. 2015.
- Ahmed, S., Nelson, P.A., Gallagher, K.G., Dees, D.W., “Energy Impact of Cathode Drying and Solvent Recovery during Lithium-ion Battery Manufacturing,” Journal of Power Sources 322 (2016) 169-178.

MATERIALS COST UPDATE

	V 3B March 2015	V 3.0 December 2015
NCA	33	24
NMC441	26	
NMC622		18
NMC333	31	20
LMO	10	10
$x\text{LMO} + (1-x)\text{NMC}$		Calculated
Negative Active (Graphite)	19	15

BATPAC DESIGNS THE BATTERY AND CALCULATES ITS MASS, VOLUME, MATERIALS, HEAT TRANSFER NEEDS, AND COST

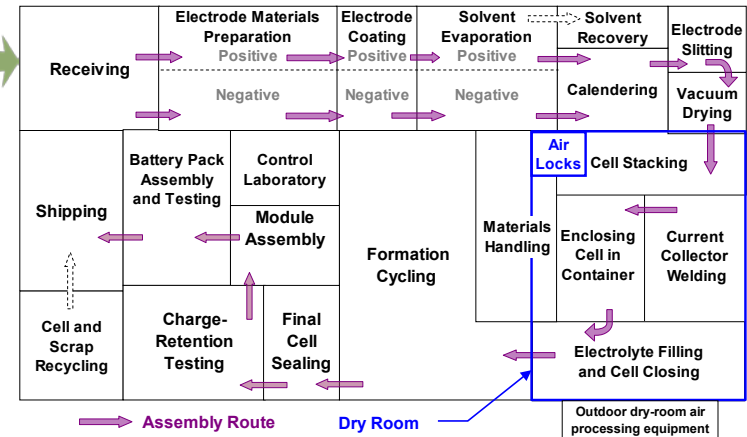
Iterate Over Governing Eqs. & Key Design Constraints

- Cell, module, & pack format
- Maximum electrode thickness
- Fraction of OCV at rated power

Battery Pack Components

- Volume
- Mass
- Materials
- Heat generation

$$\text{Process cost} = \text{Baseline cost} \cdot \left(\frac{\text{Processing rate}}{\text{Baseline processing rate}} \right)^p$$



• Pack specifications

- Power and energy (range)
- Number of cells

• Cell Chemistry

- Area-specific impedance (ASI)
- Reversible capacity C/3
- OCV as function of SOC
- Physical properties

Governing Equations

$$E = N \cdot C \cdot \left(U_E - \frac{C}{3} \frac{ASI_E}{A} \right)$$

$$L = \frac{C}{Q \cdot \rho \cdot \epsilon \cdot A}$$

$$I = \frac{P}{A \cdot N \cdot U_p \left[\frac{V}{U} \right]}$$

$$A = \frac{ASI_p \cdot P}{N \cdot (U_p)^2 \left[\frac{V}{U} \right] \left(1 - \left[\frac{V}{U} \right] \right)}$$

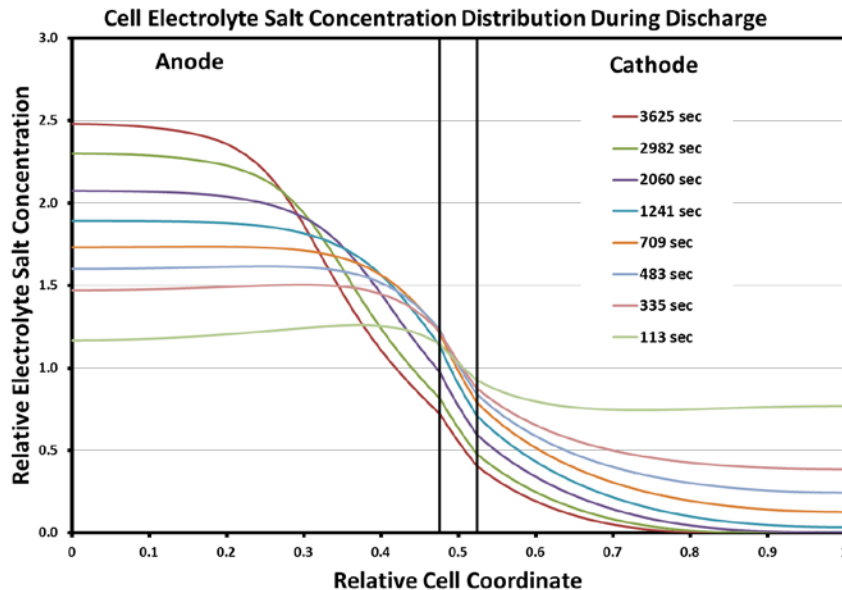
$$ASI = \frac{\alpha + f(I)}{L} + \beta$$

Total Cost to OEM

- Materials & purchased items
- Individual process steps
- Overhead, depreciation, etc.
- Warranty

CHARACTERISTIC LENGTH FOR ELECTROLYTE TRANSPORT KEY TO CALCULATING OPTIMAL ELECTRODE LOADING

- Concentration gradients limit utilization of electrode capacity



NCA/Graphite Li-Ion Cell Simulation
245 μm Electrodes 1C Discharge

Electrolyte Concentrated Solution
Transport Equation

$$\varepsilon \frac{\partial c}{\partial t} = \frac{\varepsilon}{\tau} \nabla \cdot (D \nabla c) + \frac{\nabla \cdot [(1 - c \bar{V}_e)(1 - t_+^o) \vec{i}_2]}{z_+ \nu_+ F}$$

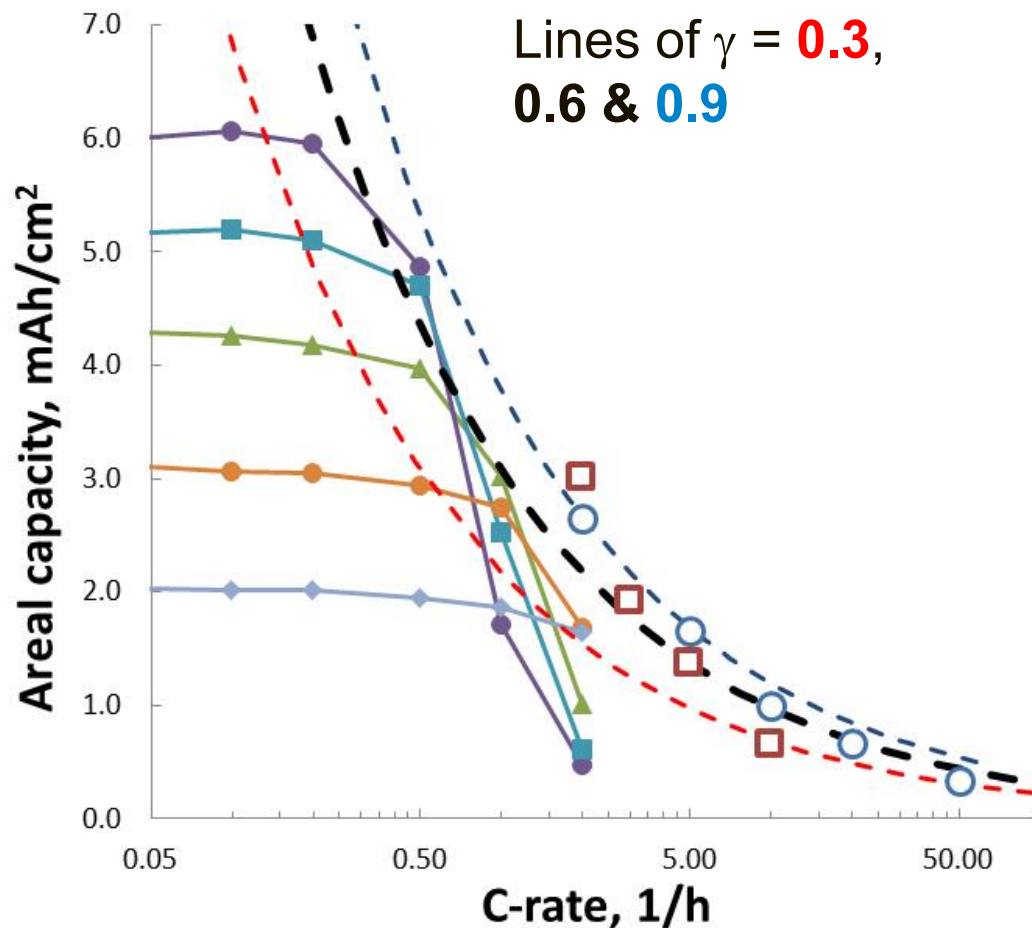
Characteristic Length, L^* , in
Porous Electrode

$$L^* = \frac{\left(\frac{\varepsilon}{\tau}\right) D c z_+ \nu_+ F}{(1 - t_+^o) I}$$

Optimal Loading as a Fraction
of Characteristic Length

$$Q_A = Q_v L = Q_v \gamma L^* = \sqrt{\frac{\gamma Q_v \left(\frac{\varepsilon}{\tau}\right) D c z_+ \nu_+ F t_d}{(1 - t_+^o)}}$$

DESIGNING MAXIMUM ELECTRODE LOADING BY RATE REQUIRED FOR CONSTANT DISCHARGE



For these tested electrodes
NMC622/Graphite (closed symbols)

Continuous C-rate	Design capacity, mAh/cm ²
C/5	4.8
C/3	3.8
C/2	3.1
1C	2.1
2C	1.5
3C	1.25

Designs should target electrode thicknesses of $\sim 0.3L^*$ or less at required C-rate

Open symbols transformed from: Zheng et al *Electrochim. Acta* 71 (2012) 258 [blue LFP/Gr & red NMC333/Gr]